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14. ABSTRACT

Basic plasma science plays an increasingly significant role in applications of importance to the United States Air Force. Many of these applications require a fully kinetic description in at least part of the domain. The most common approach is to use a fully Lagrangian framework, where the model is reduced to tracking the evolution of test particles in phase space. Of the many varieties, the most accepted approach is Particle-In-Cell. The PI, with his collaborators, is developing an alternative approach, the Boundary Integral Treecode (BIT). BIT is based on fast summation algorithms and boasts arbitrary accuracy. In a range of numerical experiments, the all scale resolution of BIT has proven to provide a substantial improvement over PIC. A major objective in this currant work is to develop a grid-free electromagnetic formulation of BIT.

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Grid-Free Electromagnetic Particle Simulations

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Abstract Basic plasma science plays an increasingly significant role in applications of importance to the United States Air Force. Many of these applications require a fully kinetic description in at least part of the domain. The most common approach is to use a fully Lagrangian framework, where the model is reduced to tracking the evolution of test particles in phase space. Of the many varieties, the most accepted approach is Particle-In-Cell [1]. The PI, with his collaborators, is developing an alternative approach, the Boundary Integral Treecode (BIT) [2]. BIT is based on fast summation algorithms and boasts arbitrary accuracy. In a range of numerical experiments, the all scale resolution of BIT has proven to provide a substantial improvement over PIC [2]. A major objective in this currant work is to develop a grid-free electromagnetic formulation of BIT.

Summary Over the past four years, while developing our methodology for a grid-free electromagnetic formulation of BIT, several significant topics, which need to be addressed, have become central in our research efforts. These include the: 1) Extended our 1D analysis of the impact of kernel regularization on the accuracy of the solution in the vicinity of boundaries to 3D (in preparation [8]- Dr. Christlieb, Dr. Cartwright and Dr. Ong), 2) worked on development of Boundary Integral Corrected PIC (in preparation - Dr. Christlieb, Dr. Cartwright and Dr. Ong), 3) a multi-scale approach to time stepping of coupled stiff systems based on our high order semi-implicit integrators [3,4,5], 4) applied our parallel time integrator [6,7] to problems that to time stepping of one million particles using 3D BIT to compute fields and demonstrated that even with the problem does not fit in cash we still get 4th order in wall clock time of forward Euler (in preparation - Dr. Christlieb, Dr. MacDonald and Dr. Ong), 5) development of arbitrary order asymptotic preserving methods for multi-scale problems (under development - Dr. Christlieb), 6) development of arbitrary order adaptive methods based on explicit and semi-implicit integral differed correction (work complete - in preparation - Dr. Christlieb, Dr. MacDonald, Dr. Ong), 7) a study of the impact of regularization on solutions to the Schrodinger equation - (in preparation - Dr. Christlieb, Dr. Krasny and Dr. Ong), 8) translation and adaptation of a 3D c++ BIT code to parallel CUDA for GPU architecture (under development - Dr. Christlieb, Dr. Johnston and Dr. Ong), 9) development of implicit time stepping methods based for Maxwell's equations using the BIT metrology (currently modifying 3D BIT code to handle 3D Maxwell kernel - Dr. Christlieb, Mr. VanGroningen and Dr. Ong), 10) extension of BIT to radiative transport problems ([9]/method under development - Dr. Christlieb, Dr. Hitchon, Dr. Lawler and Dr. Lister) 11) extension to 2D of an adaptive mesh refinement framework based on WENO (Dr. Christlieb, Dr. Qiu and Dr. Shen - Goal is AMR VP solver based on WENO) [10]. All of these topics are linked by a desire to bridge the multiple spatial and temporal scales which arise in plasma problems. We now give a brief summer of the progress on our time stepping methods, analysis of BIT, extension of BIT to Maxwell's equations and our high order WENO AMR framework. At the end of this document, I have attached our relevant publications.

Integral Deferred Correction Methods The Integral Deferred Correction (IDC) framework [3,4] being developed by the PI and his collaborators, has been shown as one possible way to systematically generate high order RK methods based on a low order RK method. IDC belongs to the family of integrators known as defect correction algorithms. Given a system of the form $\frac{dy}{dt} = f(t,y)$ with $y(t_0) = y_0$, IDC works as follows: let ν_i^0 be an approximation to $y(t)$ given by a p^{th} order RK method on the time steps $t_0,\ldots,t_m$; let $\nu(t)$ be a polynomial of degree at most m passing thought the ν_i^0; define the error as $e(t) = y(t) - \nu(t)$ and the residual as $r(t) = \frac{d\nu(t)}{dt} - f(t,\nu(t))$; let $Q(t) = e(t) + \int_{t_0}^t r(\tau)d\tau$; taking the derivative of the equation for $e(t)$ and re-writhing the equation in terms of $Q(t)$, we arrive at the differential form of our IDC corrector equation,

$$\frac{dQ}{dt} = f\left(t, Q + \nu_0 + \int_{t_0}^t f(\tau,\nu(\tau))d\tau\right) - f(t,\nu(t)) \,.$$

The corrector equation is solved to correct ν_i^0 differs from other defect correction methods in that the residual does note appear in differential form, rather the integral of the residual is built into the $\frac{dQ}{dt}$ equation. This inherently makes the method more robust than standard defect correction. $\frac{dQ}{dt}$ is solved with the same p^{th} order RK method and used to compute $\nu_i^1 \leftarrow \nu_i^0 + Q_i - \int_{t_0}^{t_i} r(\tau)d\tau$. The PI, along with his current and former post docs Dr. Ong and Dr. Qiu, have show that under cretin assumptions, $r-1$ successive approximations of the corrector equation solved with a p^{th} order explicit RK method, results in a $r \times p^{th}$ order method, up to a maximum order L, which is only determined by the accuracy in the approximation of the integral residual, $\int_{t_0}^{t_i} r(\tau)d\tau$. In practice, we have used a p^{th} order implicit and semi-implicit RK in the predictor and corrector and observed the same result. Dr. Morton, together with the PI, Dr. Ong and Dr. Qiu, has extended the theoretical results in [3,4] to both implicit and semi-implicit RK methods. The PI is currently working on extending these ideas to class of semi-implicit RK methods know as Asymptoticly Preserving (AP) methods. AP methods are a systematic philosophy for time stepping of systems with stiff relaxation. Given a system with a small parameter, say the Knudson number in the collisional Boltzmann equation, AP methods are a two step proceeder for developing numerical methods that give uniform convergence to the limiting system as the small parameter goes to zero, regardless of the time step. Step one involves either mathematical modeling or a clever re-casting of the system in form where taking the limit as the small parameter goes to zero yields the 'correct' limiting behavior. For the Boltzmann equation of neutral gas dynamics, this involves scaling the system so that the diffusion limit is obtained as Knudson number goes to zero. Step two involves the development of a consistent Semi-Implicit Runge-Kutta (SIRK) schema designed to give uniform convergence as the small parameter goes to zero. Then implicit part of the SIRK method handles the stiff term, in this example the collision term, implicitly and the non stiff term, here transport, explicitly. The PI has show that the IDC framework can support the type of SIRK that shows up in an AP formulation. It remains to be shown that the new method that results from embedding the AP SIRK in an IDC framework will again be an AP method. We are in the processes of applying the IDC AP SIRK to a range of test problems to provide numerical evidence that the resulting method is indeed AP, we will then focus on rigorously showing this to be the case.

We have also focused on extending our method to a parallel time integrator. IDC differs from traditional defect correction in that the integral from of the residual is used in the formulation of

the solution, instead of the differential form of the residual. On multi-core architectures, defect correction methods become extremely attractive because each correction step can be decoupled from the prediction and prior correction steps. In so doing, the methods are able to achieve high order accuracy in the wall clock time equivalent to that of the prediction step, provided multiple cores are used for the computation. We refer to this new class of defect correction as Revisionist IDC (RIDC), which allow for the corrections to be computed in parallel. **The parallel integrator we have developed is the first integrator to leverage multi-core cpus such that the method achieves p^{th} order in the wall clock time equal to that of a single forward Euler step.**

BIT Corrected PIC The use of time depended Green's functions in a fully Lagrangian framework raises the issue of needing to track a time history for each test particle. One proposed approach to controlling the need for a time history is to make use of fixed course mesh. As a first step towards the electromagnetic case, we are exploring the use of a coarse fixed mesh for domain decomposition in electrostatic problems, where BIT is used as a sub-cell method within each PIC cell. The methods presented here differ from Particle-Particle-Particle-Mesh (P3M) in that local boundary integrals are used within each cell to provide an accurate description of the local fields within a mesh cell [6]. We demonstrate that, in 1D, regularized BIT corrected PIC substantially reduces numerical heating, even when $\Delta x \gg \lambda_D$. Because of the negative impact regularization has on the solution field near boundaries, we have developed localizations of the regularization based on Taylor expanding the 1D non-regularized greens function bout the regularized kernel and have further proven that these are convergent expansions. This provides a possible adaptive approach for dealing with regularized kernels near fixed non-periodic boundaries. Further, we expect that $\Delta x \gg \lambda_D$ should increase the efficiency of large scale PIC calculations, enhancing the capability of legacy PIC codes by adding both fidelity (less numerical heating) and efficiency (allowing more flexibility in meshing at a given level of fidelity). For a wide class of electromagnetic problems, where PIC is used, this electrostatic work is beneficial, since for stability, the mesh spacing is sufficiently small that the system looks electrostatic. In collaboration with AFRL/RDHE, the PI is working on incorporating this into ICEPIC. Below we review the analysis of 1D BIT. The analysis has just recently been extend to the 2D and 3D case.

1D BI-PIC - Regularization Near cell boundaries, the solution of regularized BIT diverges from the true solution. To understand this error, we Taylor expand the non-regularized free space Green's function about the regularized one. We establish that this expansion is rigorously convergent as the number of terms goes to infinity and used this result to formally establish error bounds at a cell boundary. In addition, this expansion has a compact form in 1D and gives a way of localizing the regularization. The convergent Taylor expansion of $G^0_{1D} = \frac{1}{2}\sqrt{(x-y)^2+d^2} - d^2$ about $(x-y)^2 + d^2$,

$$G^0_{1D}(x|y) \doteq \frac{1}{2}\left(\sum_{i=0}^{N} \frac{(-1)^{i+1}(2i-3)!!}{2^i i!}\left(-d^2\right)^i \left((x-y)^2+d^2\right)^{(1-2i)/2}\right), \tag{1}$$

where $(-1)^{i+1}(2i-3)!! \equiv (1)(1)(-1)(-3)(-5)\ldots(7-2i)(5-2i)(3-2i)$, shows up as part of the constant in the i^{th} derivative in the above Taylor expansion. Using a similar procedure for

$\frac{dG^0_{1D}(y|x)}{dx}$ gives,

$$\frac{dG^0_{1D}(x|y)}{dx} \doteq \frac{1}{2}\left(\sum_{i=0}^{N}\frac{(-1)^i(2i-1)!!}{2^i i!}\left(-d^2\right)^i(x-y)\left((x-y)^2+d^2\right)^{-(2i+1)/2}\right), \qquad (2)$$

where $(-1)^i(2i-1)!! \equiv (1)(-1)(-3)\ldots(5-2i)(3-2i)(1-2i)$. The error bounds for the integral equation with regularized field for a cell with endpoints at α and β, with potential fields given at these points, using an N term approximation for G^0_{1D}, can be written as,

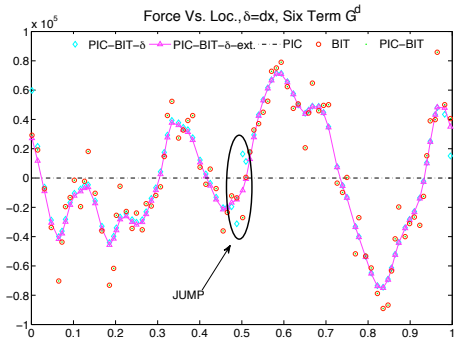
$$\begin{aligned} Err &= \frac{1}{4\sqrt{\pi}}\frac{\Gamma\left(N+\frac{1}{2}\right)}{\Gamma(N+2)}d^{2(N+1)}\int_\Omega \rho(y)\frac{d}{dx}\left[(\xi)^{-(2N+1)/2}\right]dy + \\ &\quad \int_\Omega \rho(y)\frac{d}{dx}G^d_{1D}(x|y)dy - \sum w_i\rho(x_i)\frac{d}{dx}G^d_{1D}(x|x_i)\,, \end{aligned} \qquad (3)$$

where $\xi \in ((x-y)^2,(x-y)^2+d^2)$. In equation (3), the term $\left[(\xi)^{-(2N+1)/2}\right]$ is strictly deceasing on the interval $\xi \in ((x-k)^2,(x-k)^2+d^2)$ and has its maximum value and slope at $\xi=(x-y)^2$. Hence equation (3) is bounded above by,

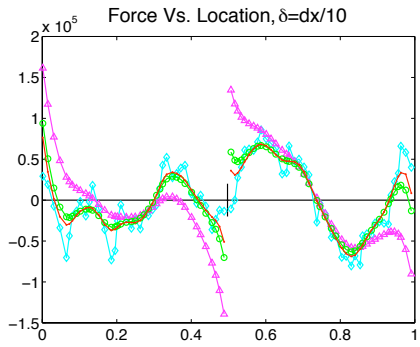
$$\begin{aligned} Err &\leq \frac{\rho_{max}}{4\sqrt{\pi}}\frac{\Gamma\left(N+\frac{1}{2}\right)}{\Gamma(N+2)}d^{2(N+1)}\left[-\frac{1}{\left((x-\beta)^2\right)^{(2N+1)/2}}+\frac{1}{\left((x-\alpha)^2\right)^{(2N+1)/2}}\right]+ \\ &\quad \int_\Omega \rho(y)\frac{d}{dx}G^d_{1D}(x|y)dy - \sum w_i\rho(x_i)\frac{d}{dx}G^d_{1D}(x|x_i)\,, \end{aligned} \qquad (4)$$

where ρ_{max} is the maximum density in the domain Ω and α and β are the end points of the domain Ω. Equation (4) agrees with our the numerical results, predicting the correct upturn at the left boundary and the correct down turn at the right boundary. Further, equation (4) demonstrates that the more localized the regularization, the closer the defect will be localized to the boundary, i.e., large N will localize the error. Figure 1 a) shows G^d_{1D} using six terms of the equations (1) and (2). It is clear that the additional terms cause the jump in PIC-BIT-δ to dramatically decrease. In addition, the interior of the cell the PIC-BIT-δ and PIC-BIT-δ-ext are in very close agreement. Further, using 6 terms in the approximation of G^0_{1D} picks up more of the features of the exact solution given by non-regularized BIT. Figure 1 b) shows the exact solution (blue diamonds) and PIC-BIT-δ with one (magenta triangles), two (green circles) and three (red dots) terms in the approximation of G^0_{1D}. It is important to note that the more localized the approximation to G^0_{1D}, the smaller the time step will need to be in the numerical simulation so as to resolve the transition in $\frac{dG^d_{1D}}{dx}$. Our work shows that the better an approximation to $\frac{dG^d_{1D}}{dx}$, the sharper the transition that needs to be resolved. So the tradeoff will be between efficiency and localization of G^d.

Time Implicit BIT Building on the idea of using the 'fixed' mesh to support a time history, the PI and Dr. Ong have developed a method of lines transpose approach to wave equations. In this case, the mesh is not a standard finite difference mesh, but rather a way of tracking the time evolution of waves not in the proximity of Lagrangian test particles. The mesh points do not have to have any uniformity to them, and could be thought of as ghost particles, which could be done with a moving mesh.



a)



b)

Figure 1: Force Vs. Location: a) PIC is the black dashed line, BIT is the green line with dots, BIT corrected PIC with $d = 0$ is the open red circles, six term G^d BIT corrected PIC with $d = \Delta x/10$ is the blue diamonds and extended cell six term G^d BIT corrected PIC is the magenta triangles. b) PIC is the black dashed line, BIT is the blue diamonds, one term G^d BIT corrected PIC with $d = \Delta x/10$ is the magenta triangles, two term G^d BIT corrected PIC with $d = \Delta x/10$ is the green circles, and three term G^d BIT corrected PIC with $d = \Delta x/10$ is the red dots.

Time Implicit BIT for Wave Type Equations: The key idea is to consider the transpose of the standard method of lines methodology, i.e., we choose to discretize in time and directly solve the resulting Helmholtz equation using an integral formulation. Observe that Maxwell's equations can be cast as

$$\frac{1}{c^2}E_{tt} - \nabla^2 E = -\mu_o J_t - \frac{1}{\varepsilon_o}\nabla\rho \ , \qquad \frac{1}{c^2}B_{tt} - \nabla^2 B = \mu_o \nabla \times J \ ,$$

where $\rho = \int f\, dv$ is the charge density, $J = \int v f\, dv$ is the current density, (ε_o, μ_o) are the permittivity and permeability and c is the speed of light. To illustrate the implicit treecode time stepping methodology for E and B, it suffices to consider the wave equation, $u_{tt} - k^2\nabla^2 u = 0$. Using a centered difference approximation to u_{tt} and evaluating $\nabla^2 u$ at time level $n+1$ gives,

$$\nabla^2 u^{n+1} - \frac{1}{k^2\Delta t^2}u^{n+1} = \frac{1}{k^2\Delta t^2}\left(-2u^n + u^{n-1}\right) \ .$$

The integral solution for u^{n+1} is

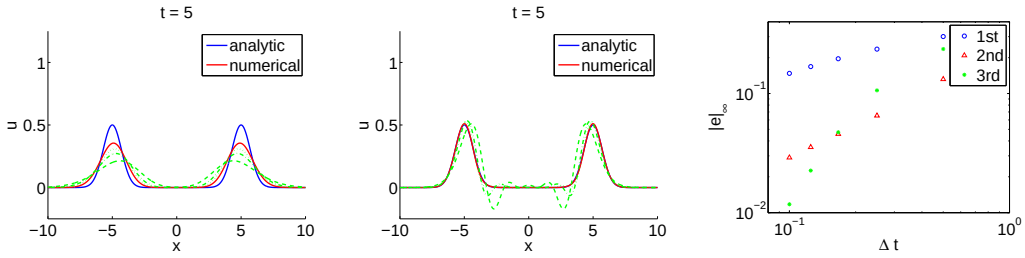
$$u^{n+1}(x) = \iint_\Omega \left(\frac{-2u^n + u^{n-1}}{k^2\Delta t^2}\right) G(x|y)\, d\Omega_y + \oint_{\partial\Omega} (u^{n+1}\nabla G - G\nabla u^{n+1})\cdot \mathbf{n}\, ds,$$

where $G(x|y)$, the free space Green's function for the Helmholtz operator $\mathcal{L}(\cdot) = (\nabla^2 - \frac{1}{k^2\Delta t^2})(\cdot)$, is $G(x|y) = \gamma\frac{exp(-r/(k\Delta t))}{r}$ in $\mathbb{R}^3$. Here, $r = ||x-y||_2$ and γ is the normalization. The volumetric and boundary integrals are approximated at the midpoints, and the resulting sums can be computed using fast summation algorithms. For the wave equation, the method is able to take time steps much larger than the imposed CFL restrictions for an explicit integrator. We have applied our approach to the wave equation in 1D, 2D and 3D with Direcltet boundary conditions. Additionally, this

implicit time stepping methodology has been extended to higher order approximations in time. Some interesting behaviors can be observed in the $\mathbb{R}^1$ simulations below. In (a), the first order scheme converges slowly to the analytic solution while in (b), the third order scheme converges much quicker, albeit with more oscillations. A convergence study is shown in (c). In this example the number of intervals used in the mid-point approximation to the volumetric integral is $M = 4000$. The initial condition is set to

$$u_o(x) = \exp(-x^2)$$

The time step used in the the implicit updates are $\Delta t = \frac{t_f}{10N}$ with $N \in \{1,2,\ldots,5\}$. Here the final time is $t_f = 5$. For all results, the analytic solution was used to start the time marching method. In each of the plots, blue curve is the exact solution, the green curves are numerical solutions with $\Delta t \in \{\frac{1}{10}, \frac{1}{20}, \frac{1}{30}\}$ and the red curves are numerical solutions with $\Delta t = \frac{1}{50}$. In all the plots we see convergence to the true solution as $\Delta t \to 0$. Observe that in all cases Δt is much larger than a cell size. Note that while in the second and third order examples display oscillations for large Δt, the oscillations rapidly deceases as Δt approaches zero, oscillations are not visible for $\Delta t = \frac{1}{50}$.



(a) first order time differencing (b) third order time differencing (c) convergence as $\Delta t \to 0$

Fast Summation: To overcome the $O(N^2)$ issue, BIT makes use of a fast summation algorithm. There are many variants of fast summation algorithms, in this case we are making use of the Treecode algorithm. The idea is to approximate the long range interaction of each distant cluster of particles as a moment expansion about the center of each cluster. Particle clusters are creates with a hierarchal tree sorting of the particles. Fields are computed using a recursive divide and conquer approach, which makes use of the tree [2].The method is $O(N \log N)$, a substantial speedup over direct summation. (Note that PIC is $O(M \log M)$ where M is the number of mesh elements.)

In the work by Lee, Johnston, and Krasny (JCP 09), a recursion relation is developed for kernels of the from $\gamma \exp(-cr)/r$. This kernel is precisely the from of the free space Green's function that arises in the 3D time implicit formulation Maxwell's equations. The recursion relation is a simple modification of the recursion relation used in electrostatic BIT and are in the processes of modifying our 3D c++ electrostatic BIT code so that we will be able to quickly develop a 3D time implicit Maxwell solver. An essential step is to consider the development of non-oscillatory time stepping methods which are higher than first order in time for the time implicit Maxwell solver.

High order AMR based on finite difference WENO As a side project, we have been working seedily to develop a high order strategy for Adaptive Meth Refinement based on Weighted Essen-

tially Non-Oscillatory finite difference methods. The new method is the first which is 3rd order in time and 5th order in space. The key ideas that have been introduced which differ from standard AMR are that the method: 1) treat refinement patches that abut one another as a singe refinement region sounded by a single ghost cell zone, 2) uses ghost cells strictly to provide boundary data to the refinement region, 3) uses Hermite interpolation to construct third order in time ghost cell data for intermediate time levels which arise in order to satisfy the CFL of the fine mesh in the refinement region, 4) uses WENO interpolation in space to provide an initial a 5th order approximation to the course soliton on the fine mesh and to update the ghost cell regions, 5) uses the WENO indicator to disced were to refine, 6) the method use a 3rd order TVD RK method to do time integration.

We have show that the method is indeed 5th order in space and 3rd order in time for smooth problems. Further, we have shown 5rd order AMR is far less diffusive than low order AMR, requiring less refinement because it is less diffusive, for a range of test problems. This include the 1D dam break problem, the 1D blast wave problem, and the 2D double Macoh refection problem. In all cases, the method give superior results, coasting less computational effort for a given accuracy than the low order AMR method.

We are working to extend these ideas to a constrained transport solver for MHD and to extend these ideas to a high order Vlasov solver.

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Publications from this work in press are all attached

3. A.J. Christlieb, B. Ong and J. Qiu, "Integral Deferred Correction Methods Constructed with High Order Runge-Kutta Methods", *AMS–Mathematics of Computation*, 79, 761–783, 2010.

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11. C. Shen, J. Qiu and A.J. Christlieb, "High Order Adaptive Mesh Refinement Based on Weighted Essentially Non-Oscillatory Schemes", *Journal of Computational Physics*, 230(10), 3780–3802, 2011

Personnel Supported by Grant

J. Qiu	Postdoc 07-08, Michigan State University
B.W. Ong	Postdoc 07-11, Michigan State University
L. VanGroningen	Student, Michigan State University
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Honors & Awards Received

Invited Speaker at IPAM 09 workshop in Quantum and Kinetic Theory – March 2009
Invited Speaker AFOSR/ONR Young Investigator Program – Oct. 2008
Air Force Young Investigator Award – awarded January 2007
NRC Summer Faculty Fellow – awarded March 2006

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Transitions

AFRL/RDHE is collaborating with the PI on transiting BIT corrected PIC into AFRL-ICEPIC.
AFRL/RDHE is collaborating with the PI on developing BIT/Gridless DSMC AFRL-CODE.

New Discoveries

Regularization at interfaces in BIT - characterized and an adaptive strategy proposed. (PI, Cartwright)
High order explicit IDC have been analyzed in terms of RK methods. (PI, Ong, Qiu)
High order explicit IDC is competitive with RK of same order (PI, Ong, Qiu)
Explicit IDC cast in parallel from ideal for multi-core technology (PI, Mac Donald, Ong)
High order semi-implicit IDC analyzed, competitive with SIRK. (PI, Morton, Ong, Qiu)
Developed implicit time stepping for wave equations with fast summation BIT framework. (PI, Ong)